Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:23 pm BST

PDB ID	:	5Q4F
Title	:	PanDDA analysis group deposition – Crystal Structure of DCLRE1A after initial refinement with no ligand modelled (structure 80)
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Deposited on	:	2017-05-25
Resolution	:	1.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

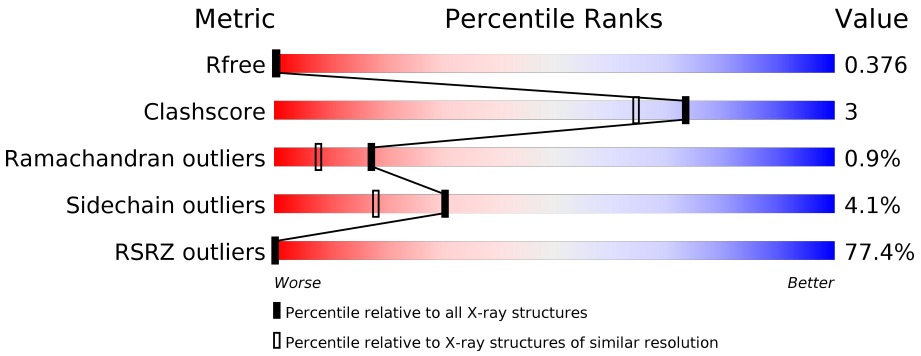
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	343	77% 86% 13% ••

2 Entry composition

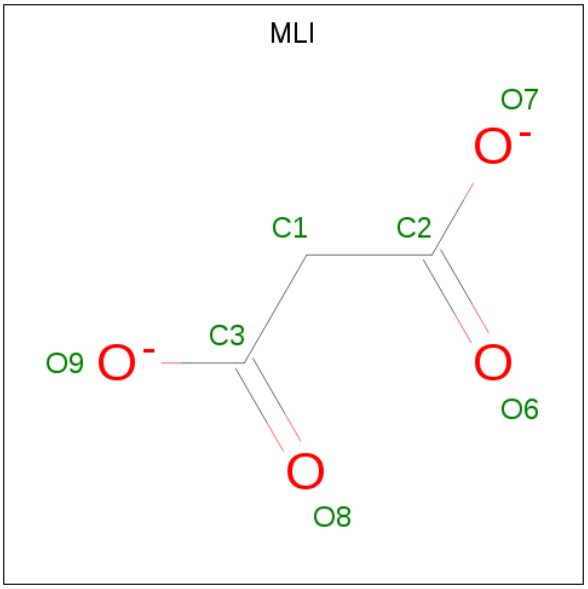
There are 4 unique types of molecules in this entry. The entry contains 3044 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DCLRE1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2726	1765	450	491	20	0	4	0

- Molecule 2 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	A	1	7	3	4		0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
3	A	1	1	1	0	0

- Molecule 4 is water.

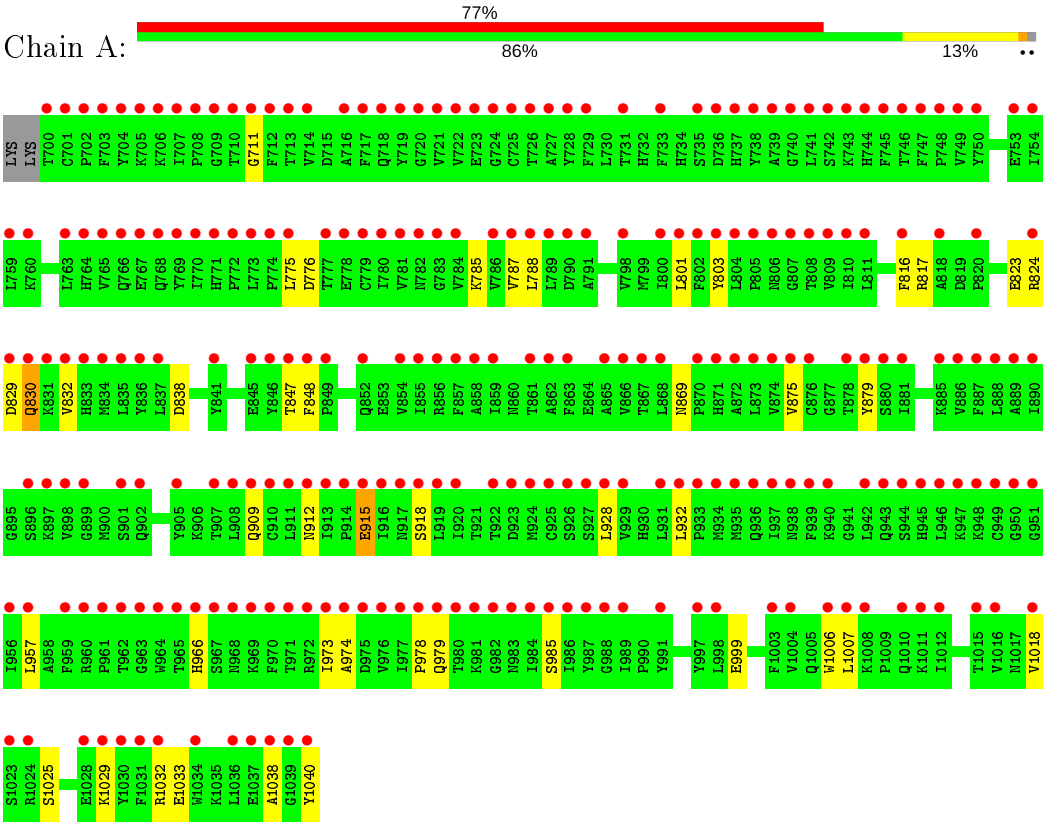
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total	O	0	0
			310	310		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DCLRE1A

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.28Å 57.44Å 115.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.56 – 1.97 57.57 – 1.97	Depositor EDS
% Data completeness (in resolution range)	94.8 (57.56-1.97) 94.8 (57.57-1.97)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.322 , 0.368 0.328 , 0.376	Depositor DCC
R_{free} test set	1193 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	2.5	Xtriage
Anisotropy	3.797	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 34.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.68	EDS
Total number of atoms	3044	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, MLI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.91	1/2802 (0.0%)	1.02	8/3809 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	999	GLU	CD-OE2	-5.22	1.20	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	838	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	817	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	A	776	ASP	CB-CG-OD1	6.44	124.09	118.30
1	A	817	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	788	LEU	CB-CG-CD1	5.43	120.23	111.00
1	A	838	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	824	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	775	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	978	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2726	0	2676	18	0
2	A	7	0	2	0	0
3	A	1	0	0	0	0
4	A	310	0	0	10	2
All	All	3044	0	2678	18	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (18) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:GLN:HB2	4:A:1441:HOH:O	1.63	0.96
1:A:909:GLN:NE2	4:A:1202:HOH:O	2.12	0.82
1:A:847:THR:HA	4:A:1425:HOH:O	1.87	0.74
1:A:1033[B]:GLU:OE2	4:A:1201:HOH:O	2.06	0.72
1:A:1029:LYS:HB2	4:A:1203:HOH:O	1.90	0.71
1:A:915:GLU:O	1:A:918:SER:OG	2.13	0.67
1:A:1029:LYS:CB	4:A:1203:HOH:O	2.44	0.66
1:A:1018:VAL:HG22	4:A:1339:HOH:O	2.00	0.61
1:A:1032:ARG:HG2	4:A:1306:HOH:O	2.10	0.49
1:A:823:GLU:HG2	1:A:1006:TRP:CD2	2.49	0.48
1:A:785:LYS:HB3	1:A:803:TYR:HB2	1.96	0.47
1:A:787:VAL:HG11	1:A:826:LEU:HD12	1.98	0.46
1:A:875:VAL:HG11	1:A:932:LEU:HD12	1.96	0.46
1:A:711:GLY:N	4:A:1205:HOH:O	2.30	0.45
1:A:1029:LYS:HB3	4:A:1203:HOH:O	2.14	0.43
1:A:832:VAL:HG21	1:A:1007:LEU:HD11	2.00	0.43
1:A:1038:ALA:HB3	1:A:1040:TYR:CE2	2.55	0.42
1:A:973:ILE:HG23	1:A:974:ALA:N	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1243:HOH:O	4:A:1248:HOH:O[3_545]	1.88	0.32
4:A:1326:HOH:O	4:A:1385:HOH:O[1_655]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	343/343 (100%)	325 (95%)	15 (4%)	3 (1%)	17 8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	966	HIS
1	A	912	ASN
1	A	915	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	299/305 (98%)	287 (96%)	12 (4%)	31 19

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	801	LEU
1	A	816	PHE
1	A	829	ASP
1	A	830	GLN
1	A	848	PHE
1	A	869	ASN
1	A	879	TYR
1	A	928	LEU
1	A	957	LEU
1	A	979	GLN
1	A	985	SER
1	A	1025	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	734	HIS
1	A	768	GLN
1	A	851	GLN
1	A	869	ASN
1	A	909	GLN
1	A	1010	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MLI	A	1101	3	0,6,6	0.00	-	0,7,7	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLI	A	1101	3	-	0/0/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	341/343 (99%)	3.18	264 (77%)	0	0	12, 25, 47, 90	0

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	970	PHE	12.0
1	A	703	PHE	9.0
1	A	971	THR	8.6
1	A	968	ASN	8.1
1	A	969	LYS	7.8
1	A	950	GLY	7.6
1	A	722	VAL	7.3
1	A	745	PHE	7.1
1	A	879	TYR	7.1
1	A	721	VAL	7.0
1	A	769	TYR	6.8
1	A	704	TYR	6.8
1	A	740	GLY	6.6
1	A	700	THR	6.3
1	A	972	ARG	6.1
1	A	748	PRO	6.0
1	A	925	CYS	6.0
1	A	702	PRO	5.9
1	A	719	TYR	5.9
1	A	765	VAL	5.8
1	A	710	THR	5.8
1	A	711	GLY	5.8
1	A	946	LEU	5.8
1	A	967	SER	5.8
1	A	781	VAL	5.7
1	A	706	LYS	5.6
1	A	739	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	701	CYS	5.6
1	A	738	TYR	5.6
1	A	829	ASP	5.5
1	A	974	ALA	5.4
1	A	949	CYS	5.3
1	A	720	GLY	5.2
1	A	937	ILE	5.2
1	A	747	PHE	5.2
1	A	726	THR	5.2
1	A	966	HIS	5.2
1	A	741	LEU	5.1
1	A	964	TRP	5.1
1	A	768	GLN	5.0
1	A	973	ILE	5.0
1	A	979	GLN	4.9
1	A	1040	TYR	4.9
1	A	965	THR	4.9
1	A	743	LYS	4.8
1	A	939	PHE	4.7
1	A	986	ILE	4.7
1	A	913	ILE	4.6
1	A	707	ILE	4.6
1	A	935	MET	4.6
1	A	770	ILE	4.5
1	A	928	LEU	4.5
1	A	872	ALA	4.5
1	A	868	LEU	4.5
1	A	782	ASN	4.4
1	A	746	THR	4.4
1	A	727	ALA	4.4
1	A	725	CYS	4.4
1	A	758	LEU	4.4
1	A	989	ILE	4.4
1	A	920	ILE	4.3
1	A	708	PRO	4.3
1	A	764[A]	HIS	4.3
1	A	808	THR	4.3
1	A	804	LEU	4.2
1	A	848	PHE	4.2
1	A	1021	TRP	4.2
1	A	870	PRO	4.2
1	A	977	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	953	TYR	4.2
1	A	780	ILE	4.1
1	A	1006	TRP	4.1
1	A	919	LEU	4.1
1	A	712	PHE	4.1
1	A	709	GLY	4.0
1	A	783	GLY	4.0
1	A	857	PHE	4.0
1	A	1018	VAL	4.0
1	A	830	GLN	3.9
1	A	728	TYR	3.9
1	A	912	ASN	3.9
1	A	763	LEU	3.9
1	A	742	SER	3.9
1	A	924	MET	3.9
1	A	878	THR	3.9
1	A	833	HIS	3.8
1	A	975	ASP	3.8
1	A	1032	ARG	3.8
1	A	846	TYR	3.8
1	A	737	HIS	3.8
1	A	874	VAL	3.8
1	A	1030	TYR	3.8
1	A	893	VAL	3.8
1	A	863	PHE	3.7
1	A	932	LEU	3.7
1	A	854	VAL	3.7
1	A	865	ALA	3.7
1	A	976	VAL	3.7
1	A	779	CYS	3.7
1	A	926	SER	3.7
1	A	987	TYR	3.7
1	A	981	LYS	3.7
1	A	805	PRO	3.7
1	A	735	SER	3.7
1	A	915	GLU	3.6
1	A	982	GLY	3.6
1	A	736	ASP	3.6
1	A	894	LEU	3.6
1	A	729	PHE	3.6
1	A	859	ILE	3.6
1	A	984	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	858	ALA	3.6
1	A	1038	ALA	3.6
1	A	826	LEU	3.6
1	A	985	SER	3.6
1	A	831	LYS	3.6
1	A	876[A]	CYS	3.6
1	A	810	ILE	3.5
1	A	873	LEU	3.5
1	A	887	PHE	3.5
1	A	803	TYR	3.5
1	A	866	VAL	3.5
1	A	917	ASN	3.5
1	A	1028[A]	GLU	3.5
1	A	802	PHE	3.5
1	A	855	ILE	3.4
1	A	773	LEU	3.4
1	A	767	GLU	3.4
1	A	856	ARG	3.3
1	A	800	ILE	3.3
1	A	750	TYR	3.3
1	A	905	TYR	3.3
1	A	916	ILE	3.3
1	A	811	LEU	3.3
1	A	942	LEU	3.3
1	A	759	LEU	3.2
1	A	766	GLN	3.2
1	A	888	LEU	3.2
1	A	836	TYR	3.2
1	A	875	VAL	3.2
1	A	956	ILE	3.2
1	A	772	PRO	3.2
1	A	849	PRO	3.2
1	A	881	ILE	3.2
1	A	980	THR	3.1
1	A	959	PHE	3.1
1	A	827	LEU	3.1
1	A	871	HIS	3.1
1	A	774	PRO	3.1
1	A	954	ASN	3.1
1	A	744	HIS	3.1
1	A	717	PHE	3.1
1	A	1031	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1034	TRP	3.1
1	A	820	PRO	3.1
1	A	1003	PHE	3.1
1	A	914	PRO	3.1
1	A	862	ALA	3.1
1	A	713	THR	3.0
1	A	962	THR	3.0
1	A	749	VAL	3.0
1	A	801	LEU	3.0
1	A	998	LEU	3.0
1	A	960	ARG	3.0
1	A	723	GLU	3.0
1	A	936	GLN	3.0
1	A	951	GLY	3.0
1	A	809	VAL	3.0
1	A	832	VAL	3.0
1	A	908	LEU	2.9
1	A	911	LEU	2.9
1	A	834	MET	2.9
1	A	943	GLN	2.8
1	A	890	ILE	2.8
1	A	880	SER	2.8
1	A	716	ALA	2.8
1	A	938	ASN	2.8
1	A	714	VAL	2.8
1	A	898	VAL	2.8
1	A	847	THR	2.8
1	A	957	LEU	2.8
1	A	754	ILE	2.8
1	A	886	VAL	2.8
1	A	775	LEU	2.7
1	A	718	GLN	2.7
1	A	755	THR	2.7
1	A	1023	SER	2.7
1	A	948	LYS	2.7
1	A	724	GLY	2.7
1	A	997	TYR	2.7
1	A	1016	VAL	2.7
1	A	784	VAL	2.7
1	A	1004	VAL	2.6
1	A	909	GLN	2.6
1	A	789	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1036	LEU	2.6
1	A	927	SER	2.6
1	A	897	LYS	2.6
1	A	1011	LYS	2.6
1	A	907	THR	2.6
1	A	902	GLN	2.6
1	A	807	GLY	2.6
1	A	771	HIS	2.5
1	A	945	HIS	2.5
1	A	1029	LYS	2.5
1	A	841	TYR	2.5
1	A	952	LYS	2.5
1	A	806	ASN	2.5
1	A	910	CYS	2.5
1	A	983	ASN	2.5
1	A	837	LEU	2.5
1	A	852	GLN	2.5
1	A	922	THR	2.5
1	A	901	SER	2.5
1	A	934	MET	2.4
1	A	777	THR	2.4
1	A	931	LEU	2.4
1	A	787	VAL	2.4
1	A	896	SER	2.4
1	A	963	GLY	2.4
1	A	1039	GLY	2.4
1	A	991	TYR	2.4
1	A	790	ASP	2.4
1	A	947	LYS	2.4
1	A	1012	ILE	2.4
1	A	818	ALA	2.3
1	A	786	VAL	2.3
1	A	1024	ARG	2.3
1	A	988	GLY	2.3
1	A	825	SER	2.3
1	A	940	LYS	2.3
1	A	731	THR	2.3
1	A	961	PRO	2.3
1	A	816	PHE	2.3
1	A	798	VAL	2.3
1	A	1037	GLU	2.3
1	A	733	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	978	PRO	2.2
1	A	923	ASP	2.2
1	A	788	LEU	2.2
1	A	944	SER	2.2
1	A	918	SER	2.2
1	A	835	LEU	2.2
1	A	791	ALA	2.2
1	A	824	ARG	2.2
1	A	867	THR	2.1
1	A	705	LYS	2.1
1	A	861	THR	2.1
1	A	899	GLY	2.1
1	A	891	ALA	2.1
1	A	1015	THR	2.1
1	A	929	VAL	2.1
1	A	1008	LYS	2.1
1	A	933	PRO	2.1
1	A	1010	GLN	2.1
1	A	885	LYS	2.1
1	A	889	ALA	2.1
1	A	1007	LEU	2.1
1	A	760	LYS	2.1
1	A	778	GLU	2.0
1	A	845	GLU	2.0
1	A	757	ASN	2.0
1	A	1020	THR	2.0
1	A	753	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MLI	A	1101	7/7	0.71	0.32	27,30,33,35	0
3	NI	A	1102	1/1	0.99	0.03	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.